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Carl L. Gardner

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13. ABSTRACT *(Maximum 200 words)*

Quantum transport effects including electron or hole tunneling through potential barriers and buildup in quantum wells are important in predicting the performance of ultra-small semiconductor devices. These effects can be incorporated into the hydrodynamic description of charge propagation in the semiconductor device.

A new extension of the classical hydrodynamic model to include quantum transport effects was derived. This "smooth" quantum hydrodynamic (QHD) model is derived specifically to handle in a mathematically rigorous way the discontinuities in the classical potential energy which occur at heterojunction barriers in quantum semiconductor devices. The smooth QHD model makes the barriers partially transparent to the particle flow and provides the mechanism for particle tunneling in the QHD model.

Smooth quantum hydrodynamic model simulations of the resonant tunneling diode were presented which exhibit enhanced negative differential resistance (NDR) when compared to simulations using the original QHD model. At both 300 K and 77 K, the smooth QHD simulations predict significant NDR even when the original QHD model simulations predict no NDR.

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The Quantum Hydrodynamic Model for Semiconductor Devices: Theory and Computations

Final Report

Carl L. Gardner

August 14, 1998

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Arizona State University

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Project Description

Quantum transport effects including electron or hole tunneling through potential barriers and buildup in quantum wells are important in predicting the performance of ultra-small semiconductor devices. These effects can be incorporated into the hydrodynamic description of charge propagation in the semiconductor device.

Refs. [1] and [2] present a new extension of the classical hydrodynamic model to include quantum transport effects. This "smooth" quantum hydrodynamic (QHD) model is derived specifically to handle in a mathematically rigorous way the discontinuities in the classical potential energy which occur at heterojunction barriers in quantum semiconductor devices. The model is valid to all orders of $\hbar^2$ and to first order in the classical potential energy.

The QHD equations have the same form as the classical hydrodynamic equations:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i}(nu_i) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}(mnu_j) + \frac{\partial}{\partial x_i}(mnu_iu_j - P_{ij}) = -n\frac{\partial V}{\partial x_j} - \frac{mnu_j}{\tau_p} \tag{2}$$

$$\frac{\partial W}{\partial t} + \frac{\partial}{\partial x_i}(u_iW - u_jP_{ij} + q_i) = -nu_i\frac{\partial V}{\partial x_i} - \frac{\left(W - \frac{3}{2}nT_0\right)}{\tau_w}. \tag{3}$$

where repeated indices are summed over and where n is the particle density, $\mathbf{u}$ is the velocity, m is the particle mass, P_{ij} is the stress tensor, V is the classical potential energy, W is the energy density, $\mathbf{q}$ is the heat flux, and T_0 is the ambient temperature. Collision effects are modeled by the relaxation time approximation, with momentum and energy relaxation times τ_p and τ_w. Quantum effects enter through the expression for the stress tensor (and for the energy density derived from the stress tensor).

Originally the quantum correction to the stress tensor in the QHD equations was given to $O(\hbar^2)$ and involved second derivatives of the classical potential.

To derive the new effective stress tensor and energy density, we construct an effective density matrix as an $O(\beta V)$ solution to the Bloch equation. Then using the effective density matrix, we take moments of the quantum Liouville equation to derive the QHD equations with the effective stress tensor and energy density [1].

The effective density matrix has the form

$$\rho(\beta,\mathbf{x},\mathbf{y}) \approx \left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} \exp\left\{-\frac{m}{2\beta\hbar^2}(\mathbf{x}-\mathbf{y})^2 - \beta\tilde{V}(\beta,\mathbf{x},\mathbf{y})\right\} \tag{4}$$

where $\tilde{V}$ is given in center-of-mass coordinates $\mathbf{R} = \frac{1}{2}(\mathbf{x}+\mathbf{y})$, $\mathbf{s} = \mathbf{x}-\mathbf{y}$ by

$$\tilde{V}(\beta,\mathbf{R},\mathbf{s}) = \frac{1}{2\beta}\int_0^\beta d\beta' \int d^3X' \left(\frac{2m\beta}{\pi(\beta-\beta')(\beta+\beta')\hbar^2}\right)^{3/2} \times$$

$$\exp\left\{-\frac{2m\beta}{(\beta-\beta')(\beta+\beta')\hbar^2}X'^2\right\}\left[V\left(\mathbf{X}'+\mathbf{R}+\frac{\beta'}{2\beta}\mathbf{s}\right)+V\left(\mathbf{X}'+\mathbf{R}-\frac{\beta'}{2\beta}\mathbf{s}\right)\right]. \tag{5}$$

Using the effective density matrix in the moment expansion of the quantum Liouville equation, we obtain the QHD conservation laws as the first three moments with

$$P_{ij} = -nT\delta_{ij} - \frac{\hbar^2 n}{4mT}\frac{\partial^2\overline{V}}{\partial x_i \partial x_j} \tag{6}$$

$$W = \frac{3}{2}nT + \frac{1}{2}mnu^2 + \frac{\hbar^2 n}{8mT}\nabla^2\overline{V} \tag{7}$$

where the "quantum potential" is

$$\overline{V}(\beta,\mathbf{x}) = \frac{1}{\beta}\int_0^\beta d\beta' \left(\frac{\beta'}{\beta}\right)^2 \int d^3X' \left(\frac{2m\beta}{\pi(\beta-\beta')(\beta+\beta')\hbar^2}\right)^{3/2} \times$$

$$\exp\left\{-\frac{2m\beta}{(\beta-\beta')(\beta+\beta')\hbar^2}(\mathbf{X}'-\mathbf{x})^2\right\} V(\mathbf{X}'). \tag{8}$$

The quantum correction to the classical stress tensor and energy density is valid to all orders of $\hbar^2$ and to first order in $\beta\,\delta V$, and involves both a smoothing integration of the classical potential over space and an averaging integration over temperature.

We define the 1D smooth effective potential in the momentum conservation equation (2) as the most singular part of $V - P_{11}$:

$$U \approx V + \frac{\hbar^2}{4mT}\frac{d^2\overline{V}}{dx^2}. \tag{9}$$

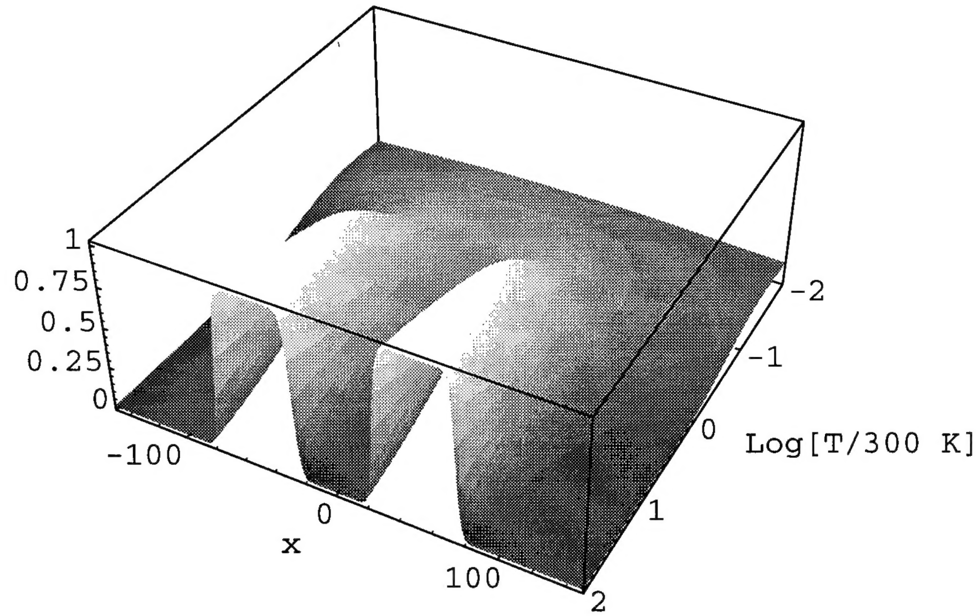

Figure 1: Smooth effective potential for electrons in GaAs for 50 Å wide unit potential double barriers and 50 Å wide well as a function of x and $\log_{10}(T/300\text{ K})$.

The double integration (over both space and temperature) provides sufficient smoothing so that the P_{11} term in the smooth effective potential actually cancels the leading singularity in the classical potential at a barrier (see Fig. 1), leaving a residual smooth effective potential with a lower potential height in the barrier region. This cancellation and smoothing makes the barriers partially transparent to the particle flow and provides the mechanism for particle tunneling in the QHD model. Note that the effective barrier height approaches zero as $T \to 0$. This effect explains in fluid dynamical terms why particle tunneling is enhanced at low temperatures. As $T \to \infty$, the effective potential approaches the classical double barrier potential and quantum effects in the QHD model are suppressed.

Smooth quantum hydrodynamic model simulations of the resonant tunneling diode were presented which exhibit enhanced negative differential resistance (NDR) when compared to simulations using the original $O(\hbar^2)$ QHD

model. At both 300 K and 77 K, the smooth QHD simulations predict significant NDR even when the original QHD model simulations predict no NDR.

The 1D steady-state smooth QHD equations are discretized [3] using a conservative upwind method adapted from computational fluid dynamics. The discretized equations are then solved by a damped Newton method.

We present simulations of a GaAs resonant tunneling diode with $Al_xGa_{1-x}As$ double barriers at 300 K (77 K). The barrier height $\mathcal{B}$ is set equal to 0.1 (0.05) eV. The diode consists of n^+ source (at the left) and drain (at the right) regions with the doping density $N_D = 10^{18}$ cm^{-3}, and an n channel with $N_D = 5 \times 10^{15}$ cm^{-3}. The channel is 200 (250) Å long, the barriers are 25 (50) Å wide, and the quantum well between the barriers is 50 Å wide. Note that the device has 50 Å spacers between the barriers and the contacts. We have chosen parameters to highlight differences between the original and smooth QHD models.

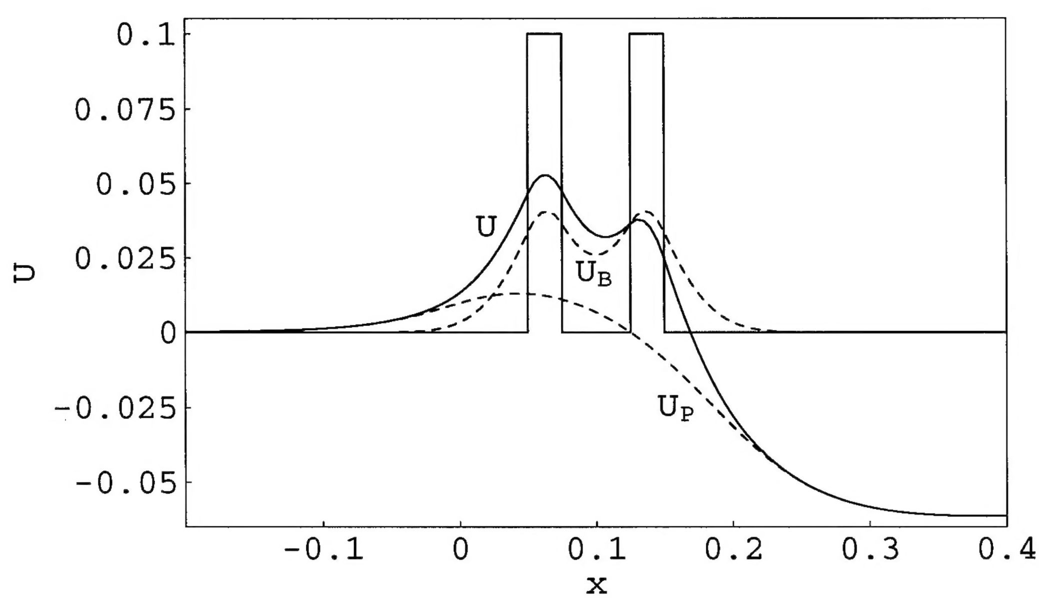

Figure 2: Smooth effective potentials U, U_B, and U_P for an applied voltage of 0.056 volts for 0.1 eV double barriers at 300 K. x is in microns.

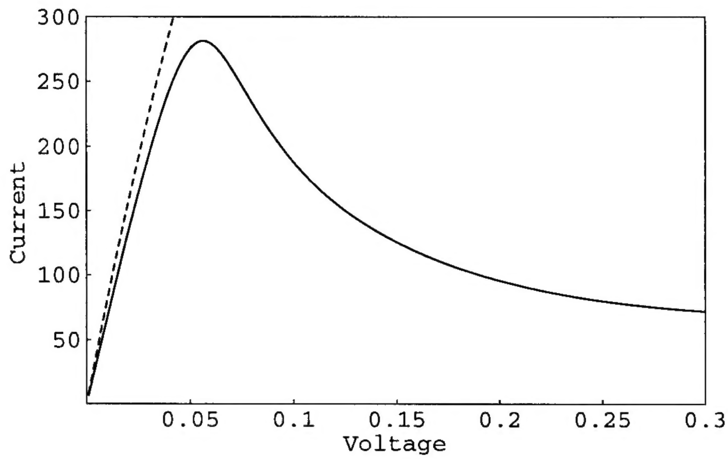

Figure 3: Current density in kiloamps/cm^2 vs. voltage for the resonant tunneling diode at 300 K. The solid curve is the smooth QHD computation and the dotted line is the $O(\hbar^2)$ computation. The barrier height is 0.1 eV.

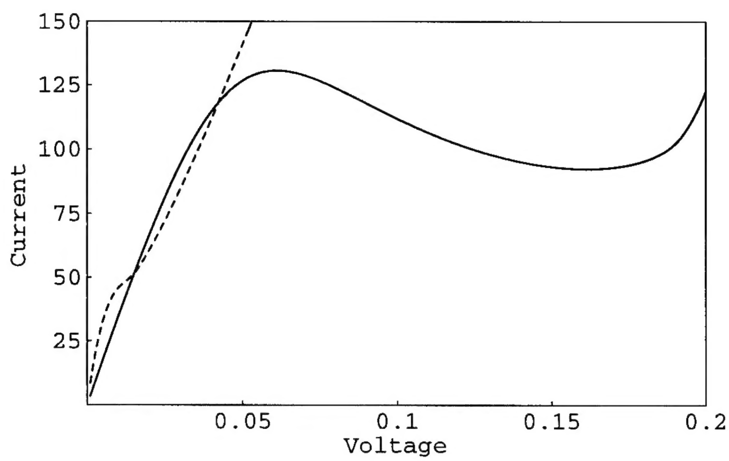

Figure 4: Current density in kiloamps/cm^2 vs. voltage for the resonant tunneling diode at 77 K. The solid curve is the smooth QHD computation and the dotted line is the $O(\hbar^2)$ computation. The barrier height is 0.05 eV.

Fig. 2 illustrates the smooth effective potentials U_B (for the barriers), U_P (the Poisson contribution), and U (barrier plus Poisson contributions) for the resonant tunneling diode at 300 K at the voltage $V = 0.056$ where the I-V curve peaks in Fig. 3.

Smooth QHD simulations of the resonant tunneling diode exhibit enhanced negative differential resistance when compared to simulations using the original $O(\hbar^2)$ QHD model. The current-voltage curve for the resonant tunneling diode at 300 K is plotted in Fig. 3 and at 77 K is plotted in Fig. 4. It is interesting that the original $O(\hbar^2)$ QHD model (see Refs. [4, 3] and references therein) predict very different I-V curves—in fact, at both 300 K and 77 K the original $O(\hbar^2)$ QHD model fails to produce negative differential resistance for these devices.

In his lectures on *Statistical Mechanics* [5], Feynman derives an effective quantum potential by a Gaussian smoothing of the classical potential. After demonstrating that the effective free energy based on the effective potential is accurate for smooth classical potentials like the anharmonic oscillator, he goes on to say that "it fails in its present form when the [classical] potential has a very large derivative as in the case of hard-sphere interatomic potential"—or for potential barriers in quantum semiconductor devices. In this investigation, we have discussed an extension of Feynman's ideas to a smooth effective potential for the quantum hydrodynamic model that is valid for the technologically important case of potentials with discontinuities.

Publications Resulting from this Grant

"Smooth Quantum Potential for the Hydrodynamic Model," C. L. Gardner and C. Ringhofer, *Physical Review* **E 53** (1996) 157–167.

"The Quantum Hydrodynamic Smooth Effective Potential," C. L. Gardner and C. Ringhofer, *VLSI Design* **6** (1998) 17–20.

"Approximation of Thermal Equilibrium for Quantum Gases with Discontinuous Potentials and Application to Semiconductor Devices," C. L. Gardner and C. Ringhofer, *SIAM Journal on Applied Mathematics* **58** (1998) 780–805.

"Smooth QHD Simulation of the Resonant Tunneling Diode," C. L. Gardner and C. Ringhofer, accepted for publication in *VLSI Design* (1998).

"Numerical Simulation of the Smooth Quantum Hydrodynamic Model for Semiconductor Devices," C. L. Gardner and C. Ringhofer, accepted for publication in *Computer Methods in Applied Mechanics* (1999).

"Theory and Simulation of the Smooth Quantum Hydrodynamic Model," C. L. Gardner, accepted for publication in *VLSI Design* (1999).

Participating Scientific Personnel

An M.A. student Andy Niemic was supported by this grant. He should obtain his M.A. in Mathematics from Arizona State University in December 1998.

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